

10781442c.trn

NEW 1

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 3 MAR 16 CASREACT coverage extended
NEWS 4 MAR 20 MARPAT now updated daily
NEWS 5 MAR 22 LWPI reloaded
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 10 APR 30 CA/CAPplus enhanced with 1870-1889 U.S. patent records
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN
NEWS 12 MAY 01 New CAS web site launched
NEWS 13 MAY 08 CA/CAPplus Indian patent publication number format defined
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 17 MAY 21 CA/CAPplus enhanced with additional kind codes for German patents
NEWS 18 MAY 22 CA/CAPplus enhanced with IPC reclassification in Japanese patents
NEWS 19 JUN 27 CA/CAPplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29 STN Viewer now available
NEWS 21 JUN 29 STN Express, Version 8.2, now available
NEWS 22 JUL 02 LEMBASE coverage updated
NEWS 23 JUL 02 LMEDLINE coverage updated
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names
NEWS 25 JUL 02 CHEMCATS accession numbers revised
NEWS 26 JUL 02 CA/CAPplus enhanced with utility model patents from China

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation

10781442c.trn

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:11:14 ON 12 JUL 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 14:11:20 ON 12 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4
DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

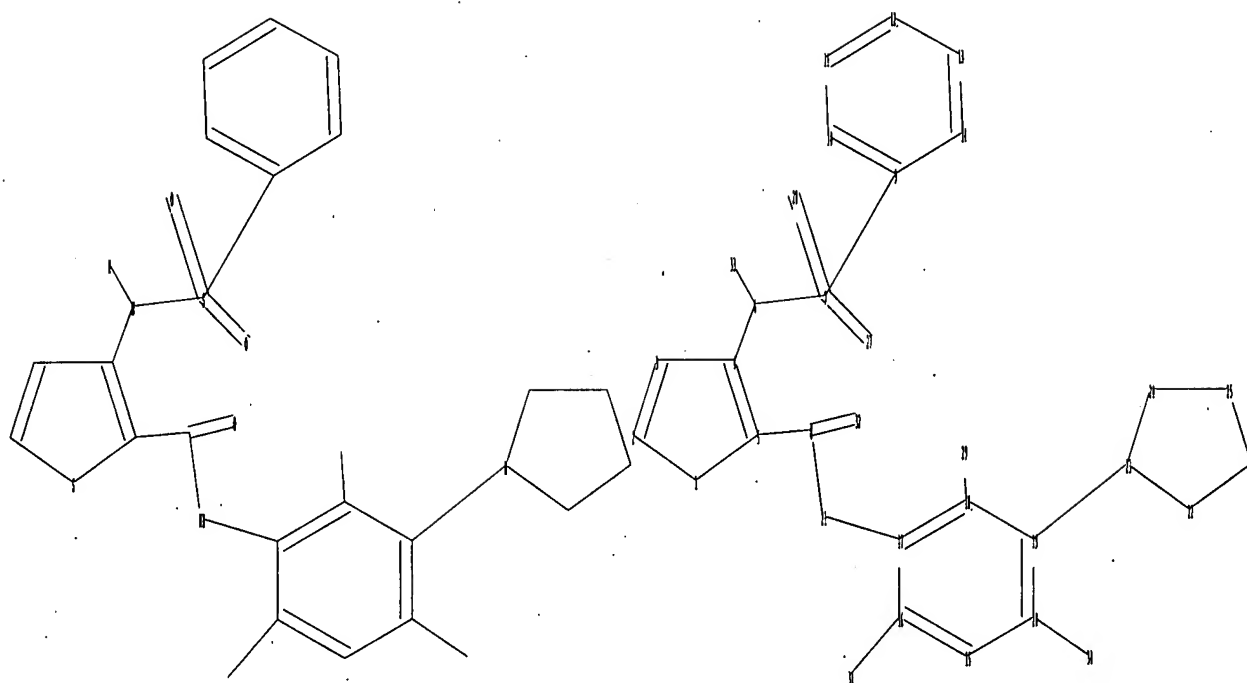
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10781442c.str



chain nodes :

6 7 8 21 27 28 29 30 31 32 33

ring nodes :

1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20 22 23 24 25 26

chain bonds :

4-6 5-8 6-7 6-33 7-9 7-27 7-28 8-21 8-32 16-31 17-21 18-29 19-23 20-30

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20
16-17 17-18 18-19 19-20 22-23 22-26 23-24 24-25 25-26

exact/norm bonds :

4-6 6-7 7-9 7-27 7-28 8-21 8-32 17-21 19-23 22-23 23-24

exact bonds :

1-2 1-5 2-3 3-4 4-5 5-8 6-33 16-31 18-29 20-30 22-26 24-25 25-26

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 9 : 15 : 22 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L1 STRUCTURE UPLOADED

=> d 11

10781442c.trn

L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:12:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 25 TO ITERATE

100.0% PROCESSED 25 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 200 TO 800
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 14:12:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 481 TO ITERATE

100.0% PROCESSED 481 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

| | | |
|----------------------|------------|---------|
| => FIL HCAPLUS | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 172.55 | 172.76 |

FILE 'HCAPLUS' ENTERED AT 14:12:49 ON 12 JUL 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3
FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

10781442c.trn

=> s 13

L4 2 L3

=> d 14 ibib abs hitstr tot

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:185392 HCAPLUS

DOCUMENT NUMBER: 142:280229

TITLE: A preparation of urotensin II receptor antagonists and CCR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, C. Eric; Bui, Huong; Gao, Daxin; Kassir, Jamal; Li, Wen; Wang, Junmei; Biediger, Ronald; Chen, Jie; Market, Robert V.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 781,442.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

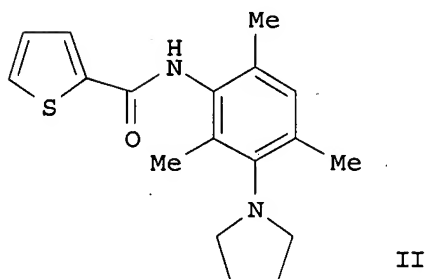
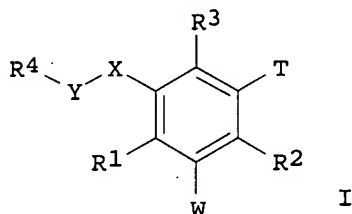
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 2005049286 | A1 | 20050303 | US 2004-924180 | 20040823 |
| US 2004180892 | A1 | 20040916 | US 2004-781442 | 20040218 |
| PRIORITY APPLN. INFO.: | | | US 2003-448791P | P 20030220 |
| | | | US 2004-781442 | A2 20040218 |

OTHER SOURCE(S): MARPAT 142:280229

GI



AB The invention relates to a preparation of urotensin II receptor antagonists and CCR-9 antagonists of formula I [wherein: R1, R2, and R3 are independently

selected from H, halogen, alkyl, aryl, or CN, etc.; X is CH₂, O, or NH, etc.; Y is SO₂, C(O), CH₂SO₂, NHC(O), or NHSO₂, etc.; T and W are independently selected from H, (cyclo)alkyl, alkoxy, aryl, or halogen, etc.; R₄ is aryl, heterocyclyl, or cycloalkyl]. For instance, thiophenecarboxamide derivative II was prepared via amidation of thiophene-2-carboxylic acid by [2,4,6-trimethyl-3-(pyrrolidin-1-yl)phenyl]amine. The invention compds. were tested for inhibition of human urotensin II-induced Ca²⁺ mobilization in UTR cells (IC₅₀ > 0.5 μM).

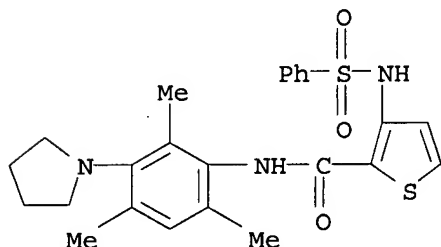
IT 749268-38-0P 847414-30-6P 847414-31-7P
 847414-33-9P 847414-34-0P 847414-35-1P
 847414-36-2P 847414-37-3P 847414-38-4P
 847414-39-5P 847414-40-8P 847414-41-9P
 847414-42-0P 847414-43-1P 847414-44-2P
 847414-45-3P 847414-46-4P 847414-47-5P
 847414-48-6P 847414-49-7P 847414-50-0P
 847414-51-1P 847414-52-2P 847414-53-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of urotensin II receptor antagonists and CCR-9 antagonists)

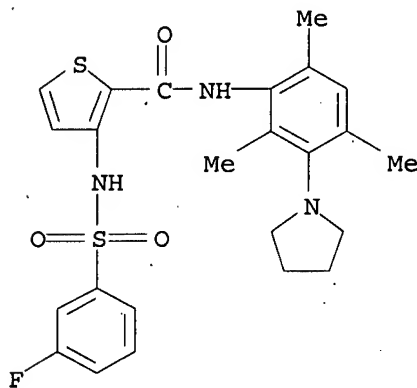
RN 749268-38-0 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(phenylsulfonyl)amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-30-6 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3-fluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

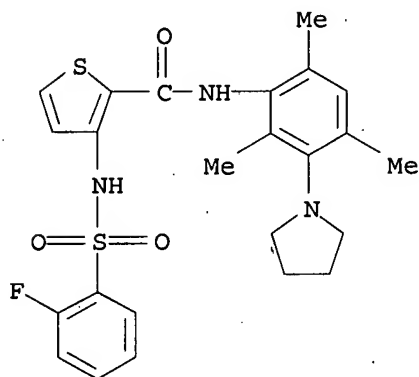


RN 847414-31-7 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(2-fluorophenyl)sulfonyl]amino]-N-[2,4,6-

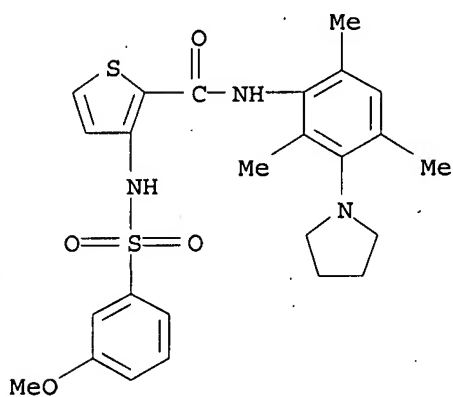
10781442c.trn

trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



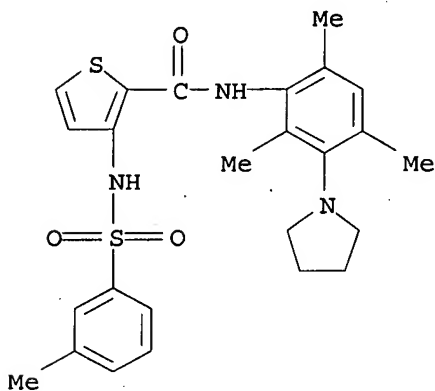
RN 847414-33-9 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3-methoxyphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



RN 847414-34-0 HCAPLUS

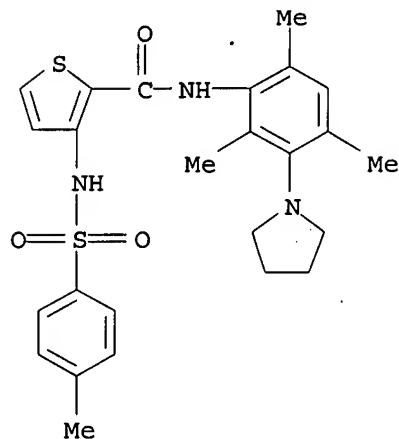
CN 2-Thiophenecarboxamide, 3-[[[(3-methylphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



10781442c.trn

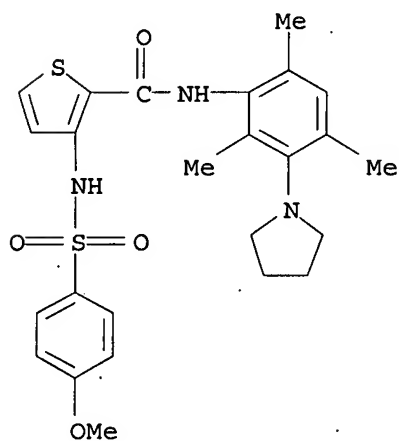
RN 847414-35-1 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(4-methylphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



RN 847414-36-2 HCAPLUS

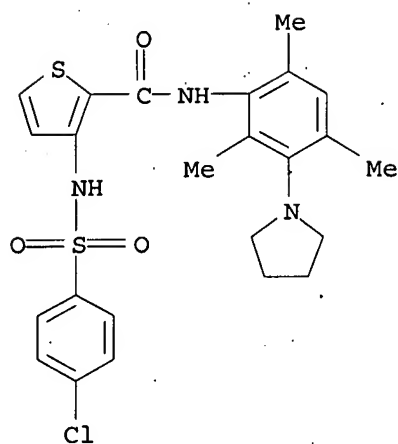
CN 2-Thiophenecarboxamide, 3-[[[(4-methoxyphenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



RN 847414-37-3 HCAPLUS

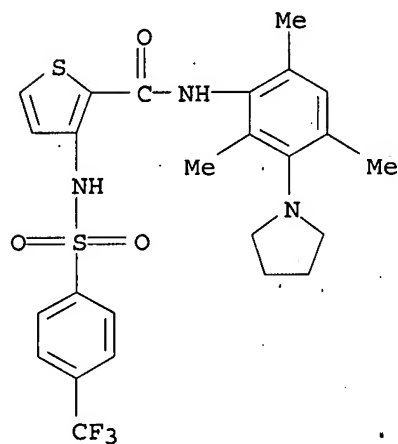
CN 2-Thiophenecarboxamide, 3-[[[(4-chlorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)

10781442c.trn



RN 847414-38-4 HCAPLUS

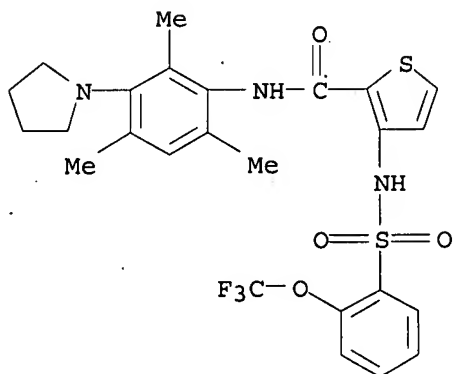
CN 2-Thiophenecarboxamide, 3-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-39-5 HCAPLUS

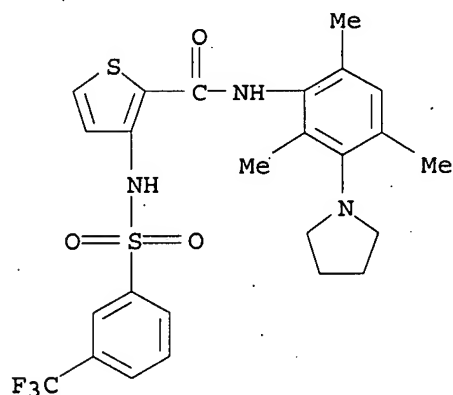
CN 2-Thiophenecarboxamide, 3-[[[2-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

10781442c.trn



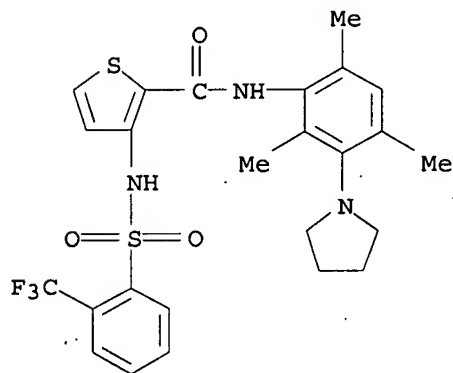
RN 847414-40-8 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



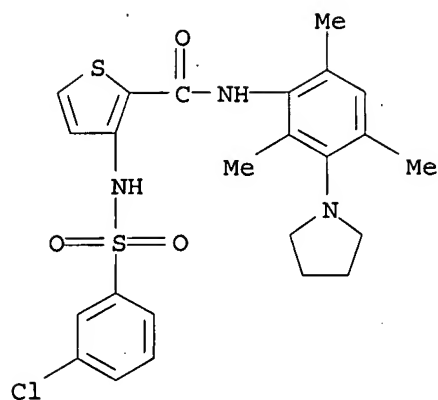
RN 847414-41-9 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[2-(trifluoromethyl)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

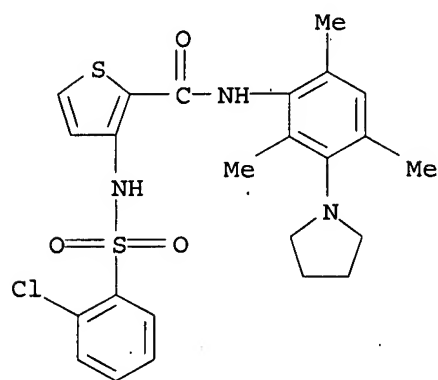


RN 847414-42-0 HCAPLUS

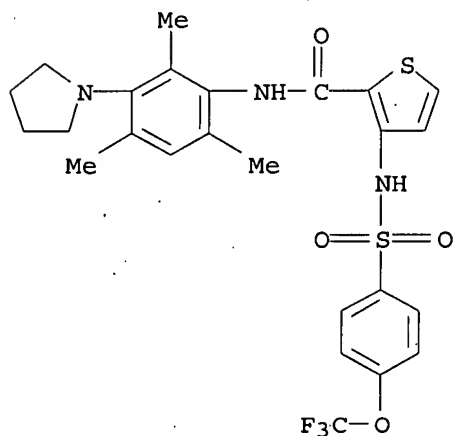
CN 2-Thiophenecarboxamide, 3-[[[3-chlorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-43-1 HCAPLUS
 CN 2-Thiophenecarboxamide, 3-[[[(2-chlorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



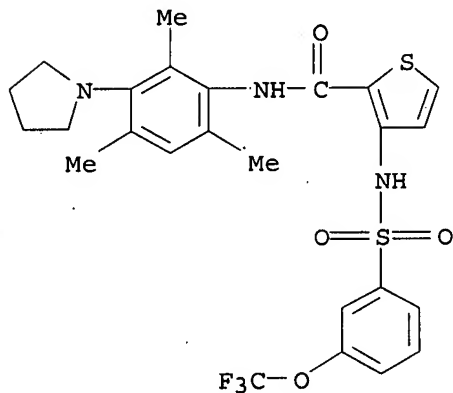
RN 847414-44-2 HCAPLUS
 CN 2-Thiophenecarboxamide, 3-[[[4-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



10781442c.trn

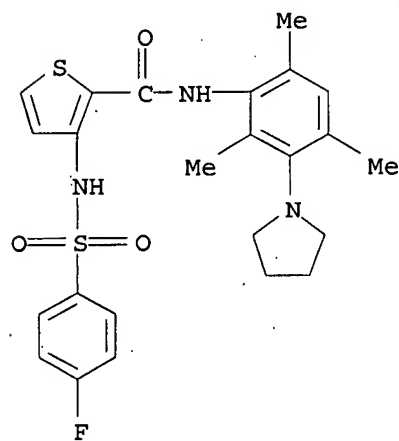
RN 847414-45-3 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[3-(trifluoromethoxy)phenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-46-4 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[4-fluorophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

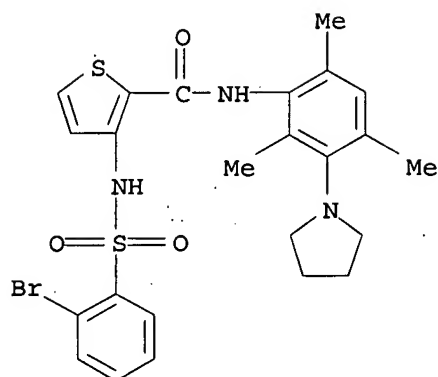


RN 847414-47-5 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[2-bromophenyl]sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

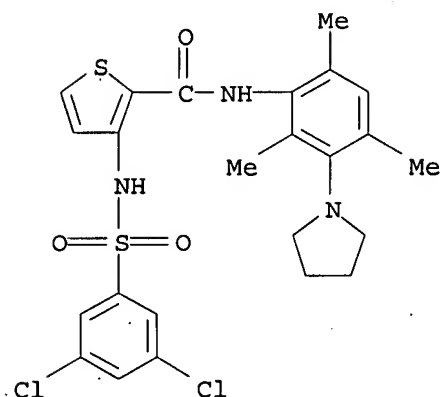


10781442c.trn



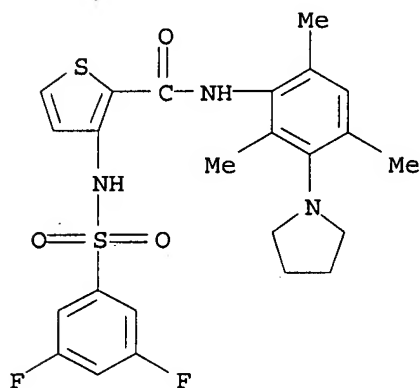
RN 847414-48-6 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3,5-dichlorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-49-7 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3,5-difluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

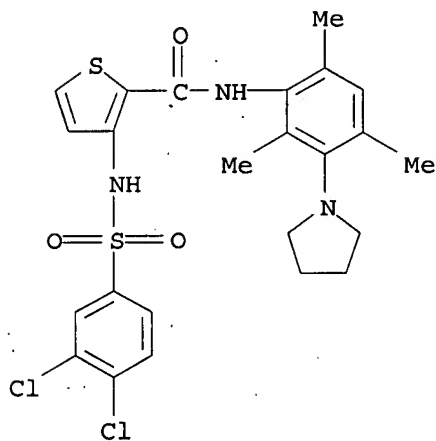


RN 847414-50-0 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3,4-dichlorophenyl)sulfonyl]amino]-N-[2,4,6-

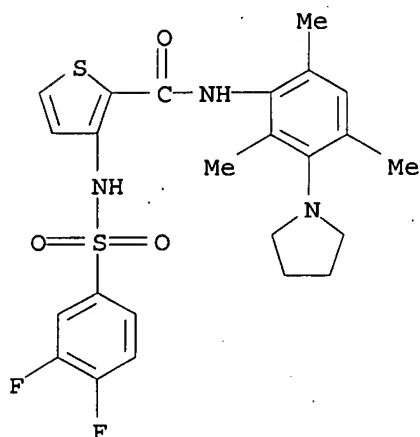
10781442c.trn

trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



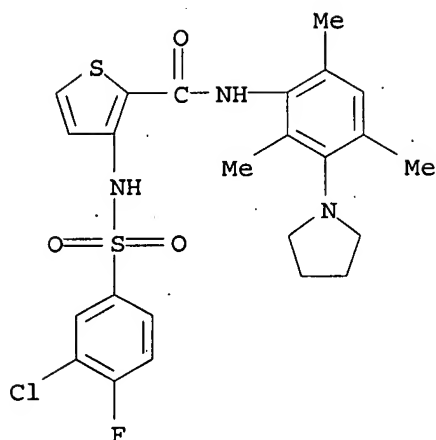
RN 847414-51-1 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3,4-difluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

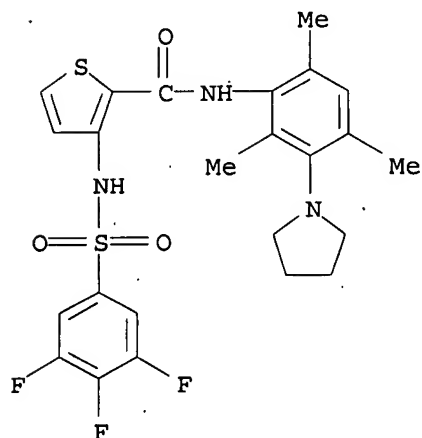


RN 847414-52-2 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(3-chloro-4-fluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

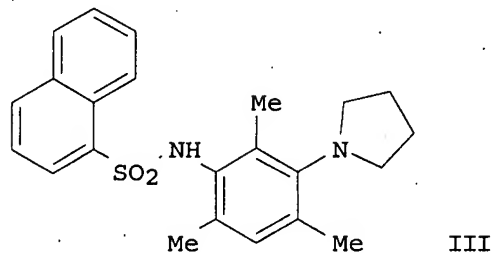
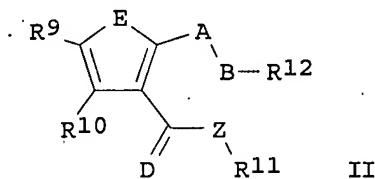
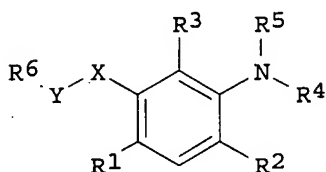


RN 847414-53-3 HCAPLUS
 CN 2-Thiophenecarboxamide, 3-[[[(3,4,5-trifluorophenyl)sulfonyl]amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:718308 HCAPLUS
 DOCUMENT NUMBER: 141:243188
 TITLE: Preparation of phenylenediamine and thiophene
 carboxylic amide derivatives as urotensin-II receptor
 antagonists and CCR-9 antagonists
 INVENTOR(S): Wu, Chengde; Anderson, Eric C.; Bui, Huong; Gao,
 Daxin; Kassir, Jamal; Li, Wen; Wang, Junmei; Market,
 Robert V.
 PATENT ASSIGNEE(S): Encysive Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 84 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|-------------------|-----------------|----------|
| WO 2004073634 | A2 | 20040902 | WO 2004-US4645 | 20040218 |
| WO 2004073634 | A3 | 20060914 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2004212985 | A1 | 20040902 | AU 2004-212985 | 20040218 |
| CA 2515780 | A1 | 20040902 | CA 2004-2515780 | 20040218 |
| EP 1610753 | A2 | 20060104 | EP 2004-712313 | 20040218 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK JP 2006519785 T 20060831 JP 2006-503636 20040218 PRIORITY APPLN. INFO.: US 2003-448791P P 20030220 WO 2004-US4645 W 20040218 | | | | |
| OTHER SOURCE(S): | | MARPAT 141:243188 | | |
| GI | | | | |



AB The title compds. I and II [R1, R2, R3 = H, halo, alkyl, aryl, aralkyl, CN, CF₃, etc.; X = N, CH₂, or O; Y = SO₂, CO, CH₂SO₂, CH₂CO, NHCO, OCO, or NHSO₂; R4 = alkyl, aralkyl or (hetero)aryl, R5 = R1, or Z-NR₇R₈, or R4, R5 taken together with N can form a 5 or 6 membered ring; Z = (CH₂)_n, where n = 0-6; R6 = (hetero)aryl, Z-NR₇R₈; R7, R8 = H, alkyl, aryl, aralkyl or together with N form a pyrrolidine, piperazine, piperidine, or morpholine ring; E = substituted amino, O, S, CR₁₃=CR₁₄, or CR₁₃=N, where, R₁₃, R₁₄ = alkyl, (hetero)aryl, halo, OH, alkoxy, etc.; D = substituted amino, O, or

S; Z = NR15 or CR15R15 where each R15 = H, alkyl, aryl, or heteroaryl; A = (substituted)amino, CO, or SO2; when A = (substituted)amino, B = SO2, CO2, or Cl6R16, where R16 = H, alkyl, aryl, or heteroaryl; when A = CO or SO2, B = (substituted)amino; R9, R10 = H, alkyl, (hetero)aryl, halo, OH, Alkoxy, or (substituted)amino; R11, R12 = H, alkyl, or (hetero)aryl] were prepared as urotensin-II receptor antagonists and CCR-9 antagonists for the treatment of congestive heart failure, stroke, ischemic heart disease, etc. For example, reaction of 2,4,6-trimethyl-3-pyrrolidin-1-yl-phenylamine (preparation given) with 1-naphthalenesulfonyl chloride yielded compound III. The latter showed an IC50 = 10 µM in the assay of human urotensin-II-induced CA2+ mobilization in UTR cells.

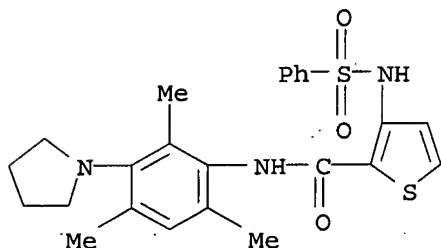
IT 749268-38-0P, 3-Benzenesulfonylamino-N-(2,4,6-trimethyl-3-pyrrolidin-1-yl-phenyl)-thiophene-2-carboxamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preparation of phenylenediamine and thiophene carboxylic amide derivs. as urotensin-II receptor antagonists and CCR-9 antagonists)

RN 749268-38-0 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(phenylsulfonyl)amino]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



=> FIL REGISTRY

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 20.94 | 193.70 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -1.56 | -1.56 |

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 14:15:30 ON 12 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

10781442c.trn

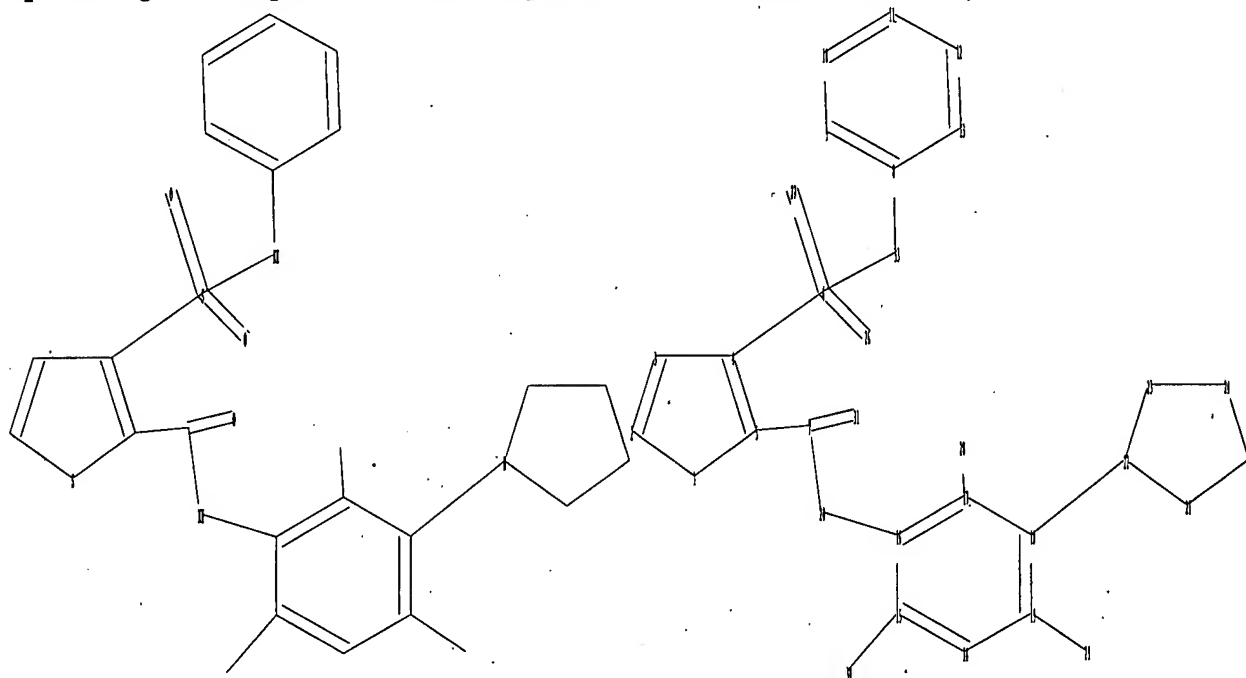
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10781442d.str



chain nodes :

6 7 20 26 27 28 29 30 31 33

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17 18 19 21 22 23 24 25

chain bonds :

4-6 5-7 6-27 6-26 6-33 7-20 7-31 8-33 15-30 16-20 17-28 18-22 19-29

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16
16-17 17-18 18-19 21-22 21-25 22-23 23-24 24-25

exact/norm bonds :

4-6 6-27 6-26 6-33 7-20 7-31 8-33 16-20 18-22 21-22 22-23

exact bonds :

1-2 1-5 2-3 3-4 4-5 5-7 15-30 17-28 19-29 21-25 23-24 24-25

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19

isolated ring systems :

containing 1 : 8 : 14 : 21 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
07/12/2007 Page 18:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 14:15:53 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 421 TO 1179

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 14:16:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 800 TO ITERATE

100.0% PROCESSED 800 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L7 4 SEA SSS FUL L5

=> FIL HCAPLUS

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 172.10 | 365.80 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.00 | -1.56 |

CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 14:16:05 ON 12 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing

10781442c.trn

of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3
FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7

L8

2 L7

=> d l8 ibib abs hitstr tot

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:185392 HCAPLUS

DOCUMENT NUMBER: 142:280229

TITLE: A preparation of urotensin II receptor antagonists and CGR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, C. Eric; Bui, Huong; Gao, Daxin; Kassir, Jamal; Li, Wen; Wang, Junmei; Biediger, Ronald; Chen, Jie; Market, Robert V.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S. Ser. No. 781,442.

CODEN: USXXCO

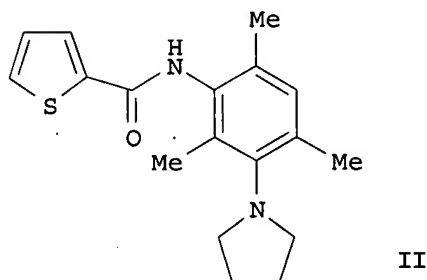
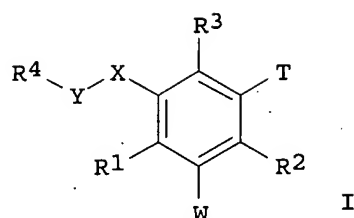
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|-------------------|-----------------|-------------|
| US 2005049286 | A1 | 20050303 | US 2004-924180 | 20040823 |
| US 2004180892 | A1 | 20040916 | US 2004-781442 | 20040218 |
| PRIORITY APPLN. INFO.: | | | US 2003-448791P | P 20030220 |
| | | | US 2004-781442 | A2 20040218 |
| OTHER SOURCE(S): | | MARPAT 142:280229 | | |
| GI | | | | |



AB The invention relates to a preparation of urotensin II receptor antagonists and CCR-9 antagonists of formula I [wherein: R¹, R², and R³ are independently selected from H, halogen, alkyl, aryl, or CN, etc.; X is CH₂, O, or NH, etc.; Y is SO₂, C(O), CH₂SO₂, NHC(O), or NHSO₂, etc.; T and W are independently selected from H, (cyclo)alkyl, alkoxy, aryl, or halogen, etc.; R⁴ is aryl, heterocyclyl, or cycloalkyl]. For instance, thiophenecarboxamide derivative II was prepared via amidation of thiophene-2-carboxylic acid by [2,4,6-trimethyl-3-(pyrrolidin-1-yl)phenyl]amine. The invention compds. were tested for inhibition of human urotensin II-induced Ca²⁺ mobilization in UTR cells (IC₅₀ > 0.5 μM).

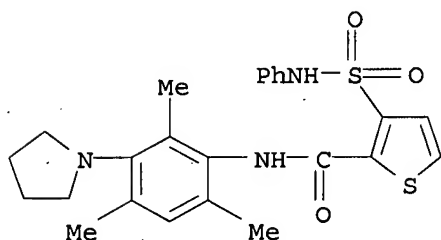
IT 749268-37-9P 847414-62-4P 847414-63-5P
847414-64-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of urotensin II receptor antagonists and CCR-9 antagonists)

RN 749268-37-9 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(phenylamino)sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

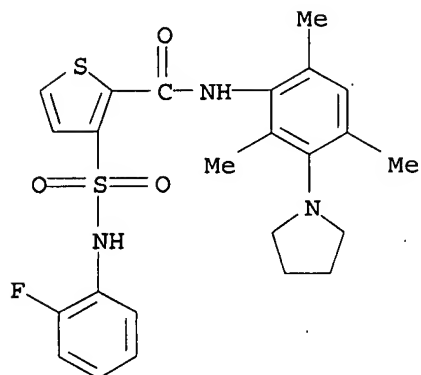


RN 847414-62-4 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[[(2-fluorophenyl)amino]sulfonyl]-N-[2,4,6-

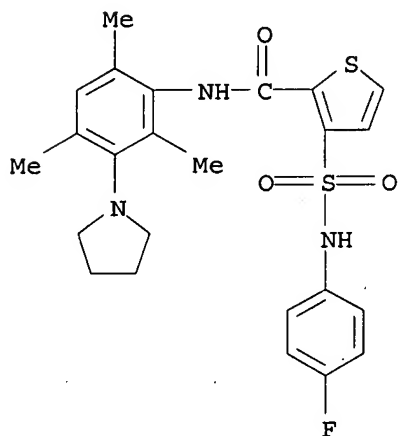
10781442c.trn

trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



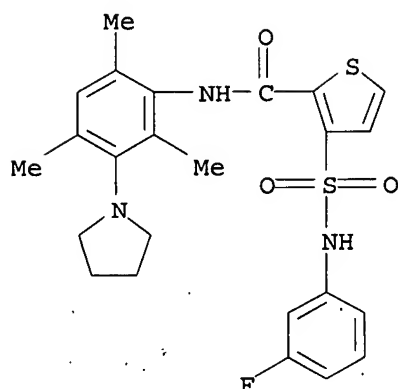
RN 847414-63-5 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[4-(4-fluorophenyl)amino]sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 847414-64-6 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[[3-(3-fluorophenyl)amino]sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:718308 HCAPLUS

DOCUMENT NUMBER: 141:243188

TITLE: Preparation of phenylenediamine and thiophene carboxylic amide derivatives as urotensin-II receptor antagonists and CCR-9 antagonists

INVENTOR(S): Wu, Chengde; Anderson, Eric C.; Bui, Huong; Gao, Maxin; Kassir, Jamal; Li, Wen; Wang, Junmei; Market, Robert V.

PATENT ASSIGNEE(S): Encysive Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

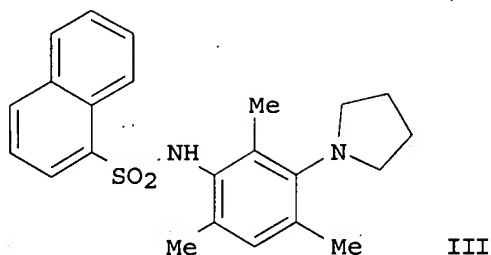
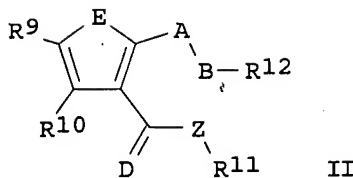
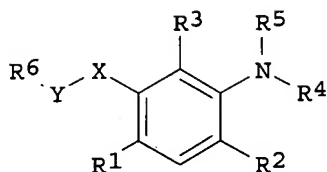
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2004073634 | A2 | 20040902 | WO 2004-US4645 | 20040218 |
| WO 2004073634 | A3 | 20060914 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2004212985 | A1 | 20040902 | AU 2004-212985 | 20040218 |
| CA 2515780 | A1 | 20040902 | CA 2004-2515780 | 20040218 |
| EP 1610753 | A2 | 20060104 | EP 2004-712313 | 20040218 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2006519785 | T | 20060831 | JP 2006-503636 | 20040218 |
| PRIORITY APPLN. INFO.: | | | US 2003-448791P | P 20030220 |
| | | | WO 2004-US4645 | W 20040218 |

OTHER SOURCE(S): MARPAT 141:243188

GI



AB The title compds. I and II [R1, R2, R3 = H, halo, alkyl, aryl, aralkyl, CN, CF3, etc.; X = N, CH2, or O; Y = SO2, CO, CH2SO2, CH2CO, NHCO, OCO, or NHSO2; R4 = alkyl, aralkyl or (hetero)aryl, R5 = R1, or Z-NR7R8, or R4, R5 taken together with N can form a 5 or 6 membered ring; Z = (CH2)_n, where n = 0-6; R6 = (hetero)aryl, Z-NR7R8; R7, R8 = H, alkyl, aryl, aralkyl or together with N form a pyrrolidine, piperazine, piperidine, or morpholine ring; E = substituted amino, O, S, CR13=CR14, or CR13=N, where R13, R14 = alkyl, (hetero)aryl, halo, OH, alkoxy, etc.; D = substituted amino, O, or S; Z = NR15 or CR15R15 where each R15 = H, alkyl, aryl, or heteroaryl; A = (substituted)amino, CO, or SO2; when A = (substituted)amino, B = SO2, CO2, or CR16R16, where R16 = H, alkyl, aryl, or heteroaryl; when A = CO or SO2, B = (substituted)amino; R9, R10 = H, alkyl, (hetero)aryl, halo, OH, Alkoxy, or (substituted)amino; R11, R12 = H, alkyl, or (hetero)aryl] were prepared as urotensin-II receptor antagonists and CCR-9 antagonists for the treatment of congestive heart failure, stroke, ischemic heart disease, etc. For example, reaction of 2,4,6-trimethyl-3-pyrrolidin-1-yl-phenylamine (preparation given) with 1-naphthalenesulfonyl chloride yielded compound III. The latter showed an IC₅₀ = 10 μM in the assay of human urotensin-II-induced CA₂⁺ mobilization in UTR cells.

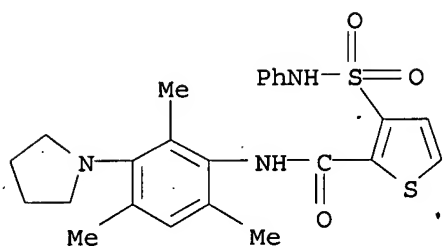
IT 749268-37-9P, 3-Phenylaminosulfonyl-N-(2,4,6-trimethyl-3-pyrrolidin-1-yl-phenyl)-thiophene-2-carboxamide
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preparation of phenylenediamine and thiophene carboxylic amide derivs. as urotensin-II receptor antagonists and CCR-9 antagonists)

RN 749268-37-9 HCAPLUS

CN 2-Thiophenecarboxamide, 3-[(phenylamino)sulfonyl]-N-[2,4,6-trimethyl-3-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

10781442c.trn



=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

26.14

391.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.56

-3.12

STN INTERNATIONAL LOGOFF AT 14:19:48 ON 12 JUL 2007

NEW 2

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 3 MAR 16 CASREACT coverage extended
NEWS 4 MAR 20 MARPAT now updated daily
NEWS 5 MAR 22 LWPI reloaded
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 10 APR 30 CA/CAPplus enhanced with 1870-1889 U.S. patent records
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN
NEWS 12 MAY 01 New CAS web site launched
NEWS 13 MAY 08 CA/CAPplus Indian patent publication number format defined
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 17 MAY 21 CA/CAPplus enhanced with additional kind codes for German patents
NEWS 18 MAY 22 CA/CAPplus enhanced with IPC reclassification in Japanese patents
NEWS 19 JUN 27 CA/CAPplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29 STN Viewer now available
NEWS 21 JUN 29 STN Express, Version 8.2, now available
NEWS 22 JUL 02 LEMBASE coverage updated
NEWS 23 JUL 02 LMEDLINE coverage updated
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names
NEWS 25 JUL 02 CHEMCATS accession numbers revised
NEWS 26 JUL 02 CA/CAPplus enhanced with utility model patents from China

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation

10781442.trn

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 13:18:39 ON 12 JUL 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:19:04 ON 12 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

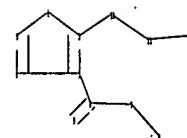
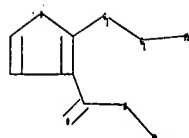
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10781442.str



chain nodes :
 6 7 8 9 10 11 12
 ring nodes :
 1 2 3 4 5
 chain bonds :
 2-10 3-6 6-7 6-9 7-8 10-11 11-12
 ring bonds :
 1-2 1-5 2-3 3-4 4-5
 exact/norm bonds :
 2-10 6-7 6-9 10-11 11-12
 exact bonds :
 1-2 1-5 2-3 3-4 3-6 4-5 7-8
 isolated ring systems :
 containing 1 :

G1:SO2,NH,N

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
 10:CLASS 11:CLASS 12:CLASS

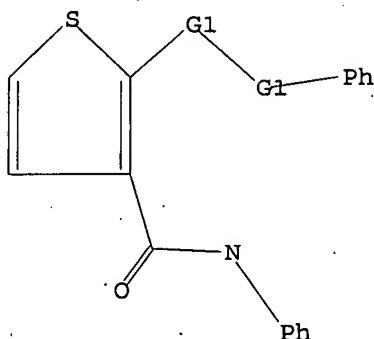
L1 STRUCTURE UPLOADED

=> D L1
 L1 HAS NO ANSWERS

10781442.trn

L1

STR



G1 SO₂,NH,N

Structure attributes must be viewed using STN Express query preparation.

=> S L1

SAMPLE SEARCH INITIATED 13:19:19 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2424 TO 3936

PROJECTED ANSWERS: 0 TO 0

L2

0 SEA SSS SAM L1

=> S L1 SSS FULL

FULL SEARCH INITIATED 13:19:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3278 TO ITERATE

100.0% PROCESSED 3278 ITERATIONS

0 ANSWERS

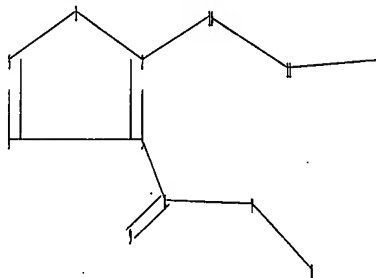
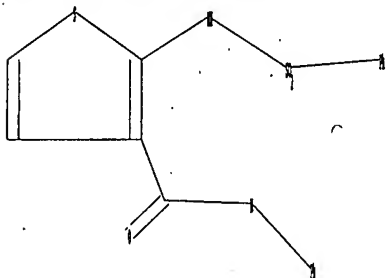
SEARCH TIME: 00.00.01

L3

0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10781442a.str



chain nodes :

6 7 8 9 10 11 12

10781442.trn

ring nodes :
1 2 3 4 5
chain bonds :
2-10 3-6 6-7 6-9 7-8 10-11 11-12
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-10 6-7 6-9 10-11
exact bonds :
1-2 1-5 2-3 3-4 3-6 4-5 7-8 11-12
isolated ring systems :
containing 1 :

G1:SO2,NH,N

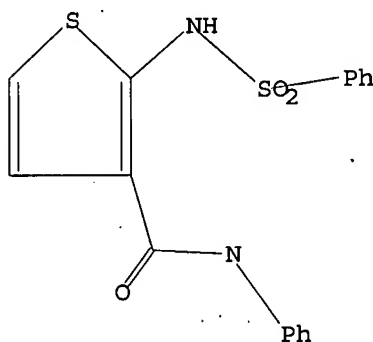
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 SO2,NH,N

Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 13:22:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 56 TO 504
PROJECTED ANSWERS: 0 TO 0

10781442.trn

L5 0 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 13:22:38 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 351 TO ITERATE

100.0% PROCESSED 351 ITERATIONS

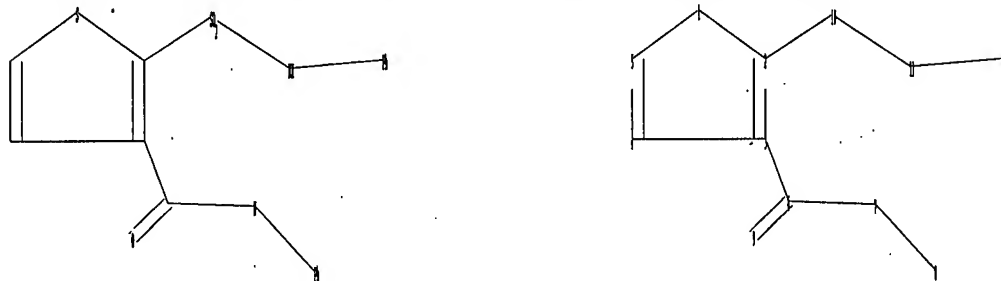
0 ANSWERS

SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\10781442b.str



chain nodes :

6 7 8 9 10 11 12

ring nodes :

1 2 3 4 5

chain bonds :

2-10 3-6 6-7 6-9 7-8 10-11 11-12

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

6-7 6-9 10-11

exact bonds :

1-2 1-5 2-3 2-10 3-4 3-6 4-5 7-8 11-12

isolated ring systems :

containing 1 :

G1:SO2,NH,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS 11:CLASS 12:CLASS

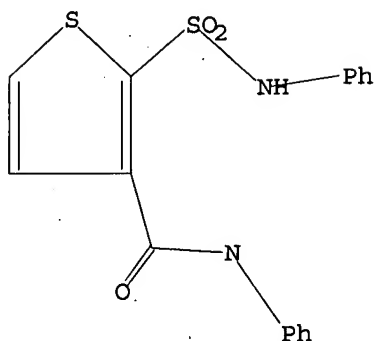
L7 STRUCTURE UPLOADED

=> d l7

L7 HAS NO ANSWERS

L7 STR

10781442.trn



G1 SO2,NH,N

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 13:24:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 13:24:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=> log y

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 519.90 | 520.11 |

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 13:25:32 ON 12 JUL 2007